

Chloroform

67-66-3 | DTXSID1020306

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 26.2 days

Global applicability domain: Outside

Local applicability domain index: 5.40e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found

Cyclopentane

Measured: 8170

Predicted: 35.5

Image not found

Benzene

Measured: 61.9

Predicted: 10.3

Image not found

Cyclohexane

Measured: 8170

Predicted: 34.7

Image not found

2,2,3-Trimethylbutane

Measured: 61.9

Predicted: 10.7

Image not found

2,3,4-Trimethylpentane

Measured: 511

Predicted: 13.9